Turkish Journal of Chemistry

Turkish Journal

of

Chemistry

Molecular Dynamics Simulation of Phase Transitions in Binary LJ Clusters

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Abstract: The structures of small clusters are studied extensively by classical simulation methods because of their interesting thermodynamic behavior. In this work, we study the thermodynamic properties of binary mixtures of noble gas atoms. Interatomic interactions are defined by 6-12 Lennard-Jones (LJ) potential. Starting from the global minimum of the potential energy surfaces, the systems are heated by increasing the total energy until melting occurs. The melting is observed by monitoring the Lindemann factor. The effects of the relative sizes of A and B atoms and the interaction strength of A-A, A-B, and B-B on the melting temperature of clusters containing 50% of each component is analyzed by using constant energy (NVE) molecular dynamics simulation. It is observed that the heterogeneous clusters melt at lower temperatures as long as the relative interactions are of similar order. Melting points do not follow a systematic trend with size, mostly due to the unusual stability of certain size clusters.

Keywords
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Turk. J. Chem., **26**, (2002), 627-640.
Full text: pdf
Other articles published in the same issue: Turk. J. Chem.,vol.26,iss.5.